

# Seminar

---

---

## Institute for Plasma Research

---

---

**Title :** Application of Carbon Nanotubes in combination with proteins for nano-delivery systems

**Speaker:** Dr. Sunita Negi  
Amity School of Applied Sciences, Haryana

**Date :** 20th May 2019 (Monday)

**Time :** 03.00PM

**Venue :** Seminar Hall, IPR

### Abstract :

Integration of carbon nanotubes with proteins is an innovative area of research because of the great application in the field of medical, nanotechnology and material science. These assemblies can act as a carrier of the drug in the case of target drug delivery. The interaction of these single walled carbon nanotube (SWCNT) with a protein would depend on the three dimensional structure of the proteins. On the other hand the chirality and the dimensions of the carbon nanotubes would also play an important role in this. The static aspect of this is concerned with how to predict the properties like structure, interforces of a protein and carbon nanotubes [1,2]. From a computational point of view, there are several main sides to this static problem: The selection of a protein and carbon nanotube and the parameter identification by VMD, NAMD [3]. A significant amount of work has been done in the past decade to reveal the unique structural, electrical, mechanical, electromechanical, and chemical properties of CNTs [4,5]. Recent research has focused on improving the quality of catalytically-produced nanotubes. Carbon nanotubes and proteins are of two different chemical natures, but their combination is going to very useful in every stream. The wide variety of functions associated with proteins has motivated a huge number of research efforts to elucidate the relationship of their biological function to their structure. Various types of biomolecules such as proteins, enzymes, or DNA/RNA can interact and be immobilized on the surface of CNTs. In this talk the speaker would give an introduction to the necessary background from physics, biophysics and surveys some of the literature. Various properties like forces, structures of combination at different environmental conditions obtained by using NAMD and VMD would also be discussed.

[1] Sunita Negi, Ayse Ozlem Aykut, Ali Rana Atilgan and Canan Atilgan, "Calmodulin Readily Switches Conformation upon Protonating High pKa Acidic Residues", *Journal of Physical Chemistry B*, 116 (24), 7145–7153 (2012).

[2] Sunita Negi, "Probing Temperature Dependent Conformation Change of Calmodulin Protein using Molecular Dynamics Simulation", *Biophysical Journal*, 108, Issue 2, Supplement 1, 46, 108 (2015).

[3] Sahil Aneja, Vivek, Kumar Bhartiya and Sunita Negi "Temperature dependent conformational studies using Molecular Dynamics Simulations", *Journal of Physics: Conference Series*, 759, 012022 (2016).

[4] Sunita Negi, Vivek Kumar Bhartiya and Shashank Chaturvedi, "Charge Calculation Studies on a Single and Double Walled Carbon Nanotube Using MOPAC", *Indian Journal of Physics* 92, 479-485 (2018).

[5] Rashmi Saini and Sunita Negi, "Charge Calculation Studies on an End-Functionalized Double Walled Carbon Nanotube using MOPAC", *Indian Journal of Physics* DOI: <https://doi.org/10.1007/s12648-019-01473-z> (2019)

---